



SPAWAR
Systems Center
San Diego

TECHNICAL REPORT 1845
December 2000

**Trace Element and
Polycyclic Aromatic
Hydrocarbon Analyses
of Jet Engine Fuels:
Jet A, JP5, and JP8**

L. A. Shumway

Approved for public release;
distribution is unlimited.

SSC San Diego

20011119 143

TECHNICAL REPORT 1845
December 2000

Trace Element and Polycyclic Aromatic Hydrocarbon Analyses of Jet Engine Fuels: Jet A, JP5, and JP8

L. A. Shumway

Approved for public release;
distribution is unlimited.



SSC San Diego
San Diego, CA 92152-5001

SSC SAN DIEGO
San Diego, California 92152-5001

Ernest L. Valdes, CAPT, USN
Commanding Officer

R. C. Kolb
Executive Director

ADMINISTRATIVE INFORMATION

The work described in this report was prepared for the Aircraft Environmental Support Office by the SSC San Diego Marine Environmental Quality Branch (D362).

Released by
J. G. Grovhoug, Head
Marine Environmental Quality Branch

Under authority of
R. H. Moore, Head
Environmental Sciences Division

S. J. Harrell, Head
Marine Environmental Support Office

J. T. Baker® is a registered trademark of the J. T. Baker Chemical Company Corporation.
Fisher Scientific® is a registered trademark of the Fisher Scientific Company.
Hewlett-Packard® is a registered trademark of the Hewlett-Packard Corporation.
Perkin-Elmer™ is a trademark of the Perkin-Elmer Corporation.
Teflon® is a registered trademark of DuPont DeNemours and Company Corporation.

EXECUTIVE SUMMARY

For this study, one sample of commercial Jet A (Jet Aviation) fuel, one sample of JP8 fuel, and two samples of JP5 fuel were analyzed for elements and Polycyclic Aromatic Hydrocarbons (PAHs). Table ES-2 is a summary of elements detected in the fuels. Shaded elements were detected at the highest concentrations. More data are needed to determine a typical composition for each fuel type.

Table ES-1. Elements detected in jet fuel.

Element	Jet A (ppb)	JP5* (ppb)	JP8 (ppb)
Aluminum	ND	2144	9360
Barium	3	9	38
Calcium	555	5256	31120
Chromium	26	9	18
Copper	5	82	6
Iron	210	210	1144
Lead	11	5	10
Magnesium	ND	1056	5840
Manganese	6	10	25
Nickel	ND	6	6
Niobium	ND	ND	2
Potassium	ND	118	207
Scandium	11	12	11
Selenium	ND	ND	21
Strontium	12	70	351
Sulfur	1220	450	1690
Tin	10	48	102
Titanium	100	35	1056
Vanadium	ND	3	18
Zirconium	16	14	39

*JP5 values shown are the higher of two JP5 sample values.

ND = No Detect

Elements not detected in any fuels were antimony, arsenic, cadmium, cobalt, gallium, gold, indium, mercury, molybdenum, palladium, platinum, rhodium, ruthenium, silver, tellurium, thallium, thorium, uranium, and zinc.

There were no high Molecular Weight (MW) PAHs in the jet fuels. In general, the higher MW PAHs biodegrade more slowly and have higher carcinogenic potential. Jet A and JP8 fuels had more PAHs than JP5 fuels. Jet A fuel had more mid-range MW PAHs than the military fuels.

This Technical Report analyzes four fuel samples. A larger data base would enable definition of a range of typical element and PAH values in jet fuel. It would also help determine which elements in the fuels are present as delivered from the refinery, or are introduced as storage and delivery system contaminants.

CONTENTS

EXECUTIVE SUMMARY	III
1. INTRODUCTION	1
2. MATERIALS AND METHODS.....	3
2.1 SAMPLE COLLECTION.....	3
2.2 LABORATORY ANALYSES	3
2.2.1 Sulfur.....	3
2.2.2 Elemental	3
2.2.3 Polycyclic Aromatic Hydrocarbons	5
3. RESULTS AND DISCUSSION.....	7
3.1 SULFUR ANALYSIS	7
3.2 ELEMENTAL ANALYSIS.....	8
3.3 POLYCYCLIC AROMATIC HYDROCARBON ANALYSIS	13
4. CONCLUSIONS AND REMARKS	19
5. BIBLIOGRAPHY	21
APPENDICES	
A. JET FUEL CHEMICAL AND PHYSICAL INFORMATION.....	A-1
B. ELEMENTAL ANALYSIS QA/QC DATA ²	B-1
C. ADL SEMIVOLATILE ORGANICS TARGET, SURROGATE, AND INTERNAL STANDARD ANALYTE LIST ³	C-1
D. QUALIFIER EXPLANATION ³	D-1

Figures

1. Fuel samples	7
2. Elements in concentrations 0 to 25 ppb in jet fuels	11
3. Elements in concentrations 25 to 400 ppb in jet fuels	11
4. Elements in concentrations >400 ppb in jet fuels	12

Tables

ES-1. Elements detected in jet fuel.....	iii
1. Fuel sulfur content.....	8
2. Elemental concentrations in jet fuel samples	9
3. Elements not detected	10
4. Comparison of jet fuel concentrations with 1997 study	13
5. PAH concentrations in jet fuels	14
6. Comparison of JP5 PAH concentrations with 1992 study	16

1. INTRODUCTION

Four samples of jet aviation fuel were collected and analyzed for a broad range of elements and Polycyclic Aromatic Hydrocarbons (PAHs). Results were compared to historical data.

One sample of commercial Jet A, two samples of JP5 fuel, and one sample of JP8 fuel were collected from four different airfields. JP8 fuel is the same basic formula as Jet A fuel, with additives for anti-icing, anti-static, and anti-corrosivity. Most U.S. Navy and U.S. Air Force airfields now stock JP8 fuel, which is less expensive (the commercial formula Jet A fuel is the base) than JP5 fuel. Shipboard detachments or locations with an increased fire hazard use JP5 fuel because it has a higher flashpoint than JP8 fuel.

Future reports will compare fuel analysis results to jet engine exhaust particulate analyses. This comparison might provide insight into how element and PAH concentrations in the fuel translate to those concentrations in the particulate exhaust after combustion.

2. MATERIALS AND METHODS

2.1 SAMPLE COLLECTION

The Jet A, JP5, and JP8 fuel samples were each collected in two 250-mL Trace Metal Free polyethylene bottles (I-CHEM N311-0250). The Fleet and Industrial Supply Center Petroleum Laboratory, San Diego, CA, analyzed one sample for sulfur. The second sample was split into two 125-mL trace-metal-free polyethylene bottles (I-CHEM N311-0125). One bottle was shipped to Arthur D. Little, Cambridge, MA, for PAH analysis. The other bottle was shipped to the Florida Institute of Technology, Melbourne, FL, for trace element analysis.

Approximately 4 liters of fuel were drained from the supply before the samples were collected. The Jet A fuel was collected from a fueling truck at Lindbergh Field, San Diego, CA. JP5 fuel samples were collected at the Marine Corps Air Station Miramar fueling depot and a Naval Air Station North Island (NASNI) fueling truck. JP8 fuel was collected from a March Air Force Reserve Base fueling truck.

2.2 LABORATORY ANALYSES

2.2.1 Sulfur

The American Society for Testing and Materials (ASTM) D-4294 Testing Method¹ was used for sulfur analysis. This test method applies to the measurement of sulfur in hydrocarbons. The applicable concentration range for this method is 0.0150 to 5.00 mass percent.

2.2.2 Elemental

The Marine and Environmental Chemistry Laboratories at the Florida Institute of Technology in Melbourne, FL, completed trace elemental analysis with Inductively Coupled Plasma Mass Spectroscopy (ICP-MS) and Flame Atomic Absorption Spectrometry (FAAS). The following methods description is summarized from their report.²

2.2.2.1 Sample Digestion (For All Elements Except Hg). Two-gram subsamples of each jet fuel were weighed directly into 50-mL Teflon[®] beakers to which 10 mL of Ultrex II nitric acid (J. T. Baker[®]) was added. The beakers were then covered with Teflon[®] watch covers and allowed to reflux gently at low heat for 24 hours. A second 10-mL aliquot of Ultrex II was then added to the beakers and the temperature increased for an additional 12 hours of vigorous refluxing. At the end of this second refluxing period, the covers were removed from the Teflon[®] beakers and the solution volume reduced to

¹ American Society for Testing and Materials. 1998. "ASTM D4294 Test Method," West Conshohocken, PA.

² "Trace Element Concentrations in Jet Fuel Samples." 1999. Technical report prepared by the Florida Institute of Technology, Marine and Environmental Chemistry Laboratories for SSC San Diego under Contract Number N66001-96-D-0050: Determination of Contaminant Levels in Environmental Samples.

~5 mL with gentle heating. The Teflon[®] beakers were then covered and allowed to cool. The digested fuel samples were transferred to graduated cylinders and brought to a final volume of 10 mL with reagent water (18-megohm resistivity) rinses of the Teflon[®] beakers. These solutions were then placed in acid-washed, 15-mL low-density polyethylene bottles for analysis.

2.2.2.2 Sample Digestion for Hg. Two-gram subsamples of each jet fuel were weighed into 50-mL glass digestion tubes and 4 mL of trace metal grade nitric acid (J.T. Baker[®] Instra-Analyzed) was added. The tubes were then covered and allowed to sit at room temperature for 3 hours to begin the digestion process. At this point, 2 mL of trace metal grade sulfuric acid (Fisher Scientific[®] TraceMetal) was added to the digestion tubes. The tubes were allowed to sit overnight (sealed) to continue digestion at room temperature. The samples were then transferred to a water bath and heated to a refluxing temperature of between 85 and 90°C for 3 hours. The digested fuel samples were allowed to cool and then transferred to graduated cylinders and brought to a final volume of 10 mL with reagent water (18-megohm resistivity) rinses of the digestion tubes. These solutions were then placed in acid-washed, 15-mL low-density polyethylene bottles for Hg analysis.

2.2.2.3 Quantitative Analysis. Jet fuel concentrations of As, Au, Ba, Cd, Ga, Mo, Ni, Pb, Pt, Sb, Sc, Sn, Sr, Ti, Tl, V, and Zr were determined quantitatively by ICP-MS using a Perkin-Elmer[™] ELAN 5000 instrument. Concentrations of Co, Cr, Cu, Fe, and Mn were determined by graphite furnace atomic absorption spectrometry (GFAAS) with a Perkin-Elmer[™] Model 4000 atomic absorption spectrometer (AAS), an HGA-400 graphite furnace, and an AS-40 autosampler. Concentrations of Ag and Se in the jet fuel were determined by GFAAS using a Perkin-Elmer[™] Model 5100PC AAS, an HGA-600 graphite furnace, and an AS-60 autosampler. Concentrations of Al, Ca, K, Mg, and Zn in jet fuel were determined by FAAS using the Perkin-Elmer[™] Model 4000 AAS. Mercury concentrations were measured by Cold-Vapor Atomic Absorption Spectrometry (CVAAS) with a Laboratory Data Control Model 1235 Mercury Monitor. In all cases, the manufacturer's specifications were followed and adherence to Quality Assurance/Quality Control (QA/QC) requirements were maintained.

A semi-quantitative scan for jet fuel concentrations of In, Nb, Pd, Rh, Ru, Te, Th, and U was conducted by ICP-MS using the ELAN5000 spectrometer in the Total Quant II mode.

2.2.2.4 QA/QC. Appendix B provides Quality Assurance and Control data. A method spike was added to one subsample of the jet fuel before digestion as a check against element loss during processing. The spiking solution contained all the elements quantitatively analyzed except Pt, which was unavailable at the time of sample digestion. The recovery of this method spike is shown as Method Spike Recovery (as percent) in the QA/QC table (appendix B). The method spike recoveries were all within accepted limits for the digestion procedures used.

Matrix spikes were prepared for two of the samples during quantitative analysis of each element. These spikes were used to check for the presence of sample matrix interferences. The results of these matrix effect checks are shown as Analytical Spike Recovery (as percent) in the QA/QC table in appendix B. The spike recoveries were all within accepted limits for the analytical procedures used.

To estimate the precision of analysis, one jet fuel sample was digested and analyzed in duplicate. The precision (reproducibility) of the analyses is shown in the QA/QC table under the heading of Analytical Precision as Relative Standard Deviation (RSD) in percent.

Fuel Standard Reference Materials (SRMs) with low-level, certified metal concentrations are unavailable. Therefore, the jet fuel analyses included samples of the SRM Trace Elements in Water

3. RESULTS AND DISCUSSION

The color of the fuel samples varied (figure 1). The JP8 fuel was olive green. Jet A fuel and JP5 fuel from Miramar were similar—a pale yellow. JP5 fuel from NASNI was dark gold. It is not known which additives and/or refining conditions cause the color variations between the samples.

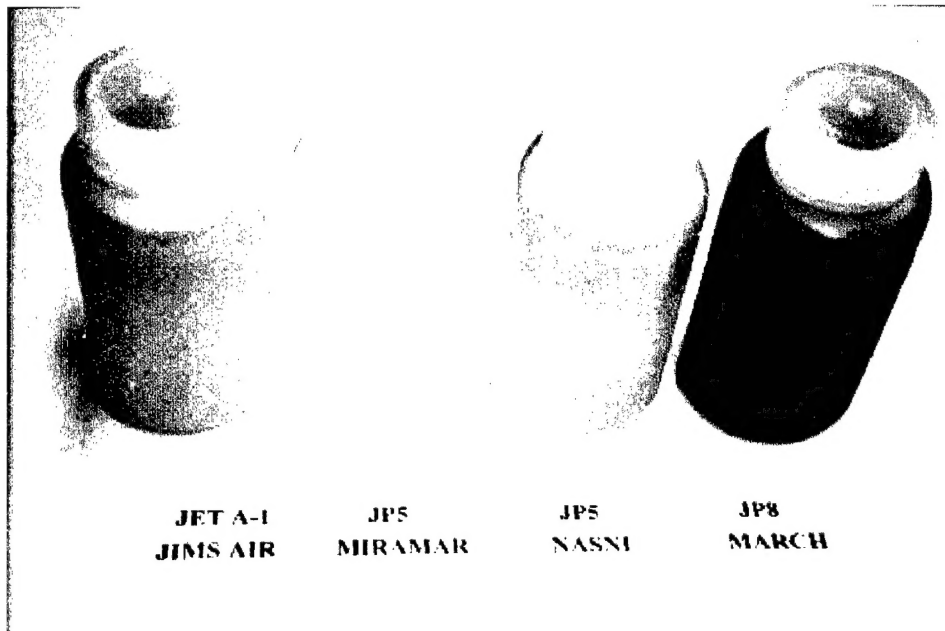


Figure 1. Fuel samples.

3.1 SULFUR ANALYSIS

Table 1 shows sulfur concentration results from testing at the Fleet and Industrial Supply Center Petroleum Laboratory, San Diego, CA. These results are compared to historical sulfur concentration data from the 1998 TRW Petroleum Technical Report, Aviation Turbine Fuels.⁴

The sulfur concentrations in this study are higher than historical values. The more recent data show sulfur concentrations are two times higher for JP5 fuel and eight times higher for JP8 fuel than the Aviation Turbine Fuels report published annually by TRW. These concentrations are notable because an average value of 0.02% sulfur has been used to calculate SO₂ emission factors for military jet engines.⁵ These emission factors may need to be reviewed, based on the higher sulfur concentrations found in this study.

⁴ C. Dickson. 1999. "Aviation Turbine Fuels." Technical report prepared for TRW Petroleum Technologies, Bartlesville, OK.

⁵ "Estimated Aircraft Engine Emissions for Center for Naval Analyses." 1997. AESO Memorandum Report No. 9731.

Table 1. Fuel sulfur content.

Fuel Type	% Sulfur by Weight in This Study		% Sulfur by Weight Aviation Turbine Fuels ⁴		
			1996	1997	1998
Jet A Lindbergh	0.1223	Min Avg Max	0.000 0.062 0.255	0.000 0.065 0.210	0.007 0.040 0.140
JP5 MCAS Miramar NASNI	0.0417 0.0472		No Data	No Data	No Data
JP8 March AFB	0.1686	Min Avg Max	0.010 0.031 0.070	0.010 0.029 0.060	0.016 0.043 0.070

3.2 ELEMENTAL ANALYSIS

Table 2 shows the elemental analysis completed at the Florida Institute of Technology using ICP-MS and FAAS.

In general, JP8 fuel had the highest elemental concentrations. With respect to the other three fuel samples, JP8 fuel had very high concentrations of aluminum, calcium, iron, magnesium, strontium, and titanium. Commercial Jet A fuel had the lowest elemental concentrations, with the exceptions of chromium, lead, and titanium.

The JP5 fuel showed significant differences in composition between those two samples for seven of the elements: aluminum, calcium, copper, magnesium, potassium, strontium, and tin. With such a limited database, it is difficult to hypothesize why there are large differences. It could be that the fuels are different as shipped from the refinery or a result of the storage or delivery system.

Table 2. Elemental concentrations in jet fuel samples.

Element	MDL ?g/L (ppb)	Jet A Lindbergh Field ?g/L (ppb)	JP5 MCAS Miramar ?g/L (ppb)	JP5 NASNI ?g/L (ppb)	JP8 March AFB ?g/L (ppb)
Aluminum	640	ND	ND	2144	9360
Antimony	2	ND	ND	ND	ND
Arsenic	4	ND	ND	ND	ND
Barium	0.5	3	4	9	38
Cadmium	1	ND	ND	ND	ND
Calcium	120	555	920	5256	31120
Chromium	2	26	9	5	18
Cobalt	2	ND	ND	ND	ND
Copper	1	5	5	82	6
Gallium	2	ND	ND	ND	ND
Gold	8	ND	ND	ND	ND
Indium*	1	ND	ND	ND	ND
Iron	4	210	210	207	1144
Lead	1	11	2	5	10
Magnesium	80	ND	ND	1056	5840
Manganese	0.5	6	4	10	25
Mercury	1	ND	ND	ND	ND
Molybdenum	2	ND	ND	ND	ND
Nickel	2	ND	5	6	6
Niobium*	1	ND	ND	ND	2
Palladium*	1	ND	ND	ND	ND
Platinum	8	ND	ND	ND	ND
Potassium	80	ND	118	ND	207
Rhodium*	1	ND	ND	ND	ND
Ruthenium*	1	ND	ND	ND	ND
Scandium	2	11	12	11	11
Selenium	16	ND	ND	ND	21
Silver	3	ND	ND	ND	ND
Strontium	2	12	17	70	351
Tellurium*	1	ND	ND	ND	ND
Thallium	4	ND	ND	ND	ND
Thorium*	1	ND	ND	ND	ND
Tin	2	10	48	6	102
Titanium	4	100	28	35	1056
Uranium*	1	ND	ND	ND	ND
Vanadium	2	ND	ND	3	18
Zinc	48	ND	ND	ND	ND
Zirconium	2	16	14	10	39

MDL = Method Detection Limit

ND = Not Detected

*= Semi-Quantitative Analysis from ICP-MS Scan

Table 3 contains elements extracted from the larger table that were not detected in at least one of the fuels. From looking at this table and referencing table 2 again, it appears the JP5 fuel at Miramar was very similar to the Jet A fuel at Lindbergh Field.

Highlighted elements in table 3 were not detected in any of the fuels.

Table 3. Elements not detected.

Element	Jet A Lindbergh Field (ppb)	JP5 MCAS Miramar (ppb)	JP5 NASNI (ppb)	JP8 March AFB (ppb)
Aluminum	ND	ND	2144	9360
Antimony	ND	ND	ND	ND
Arsenic	ND	ND	ND	ND
Cadmium	ND	ND	ND	ND
Cobalt	ND	ND	ND	ND
Gallium	ND	ND	ND	ND
Gold	ND	ND	ND	ND
Iridium	ND	ND	ND	ND
Magnesium	ND	ND	1056	5840
Mercury	ND	ND	ND	ND
Molybdenum	ND	ND	ND	ND
Nickel	ND	ND	ND	ND
Niobium	ND	ND	ND	ND
Palladium	ND	ND	ND	ND
Platinum	ND	ND	ND	ND
Potassium	ND	118	ND	207
Rhodium	ND	ND	ND	ND
Ruthenium	ND	ND	ND	ND
Selenium	ND	ND	ND	21
Silver	ND	ND	ND	ND
Tellurium	ND	ND	ND	ND
Thallium	ND	ND	ND	ND
Thorium	ND	ND	ND	ND
Uranium	ND	ND	ND	ND
Vanadium	ND	ND	3	18
Zinc	ND	ND	ND	ND

ND = No Detection

Figures 2, 3, and 4 show elemental concentrations divided into low (1 to 25 ppb), mid (25 to 400 ppb), and high (>400 ppb) concentration ranges.

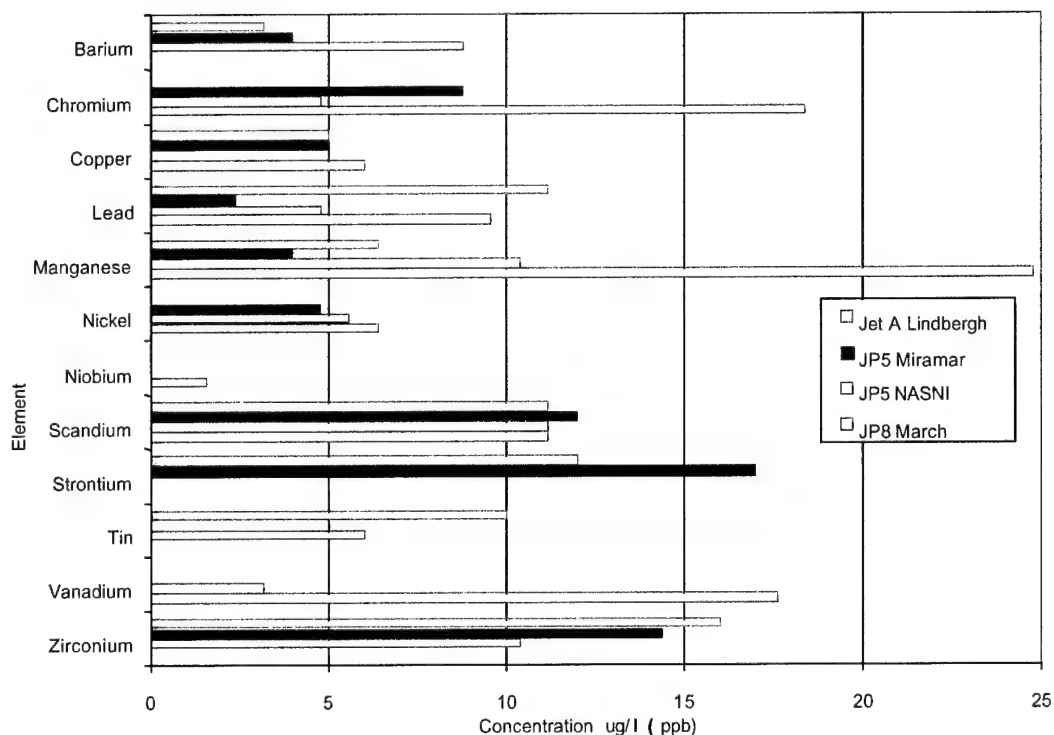


Figure 2. Elements present in concentrations 0 to 25 ppb in jet fuels.

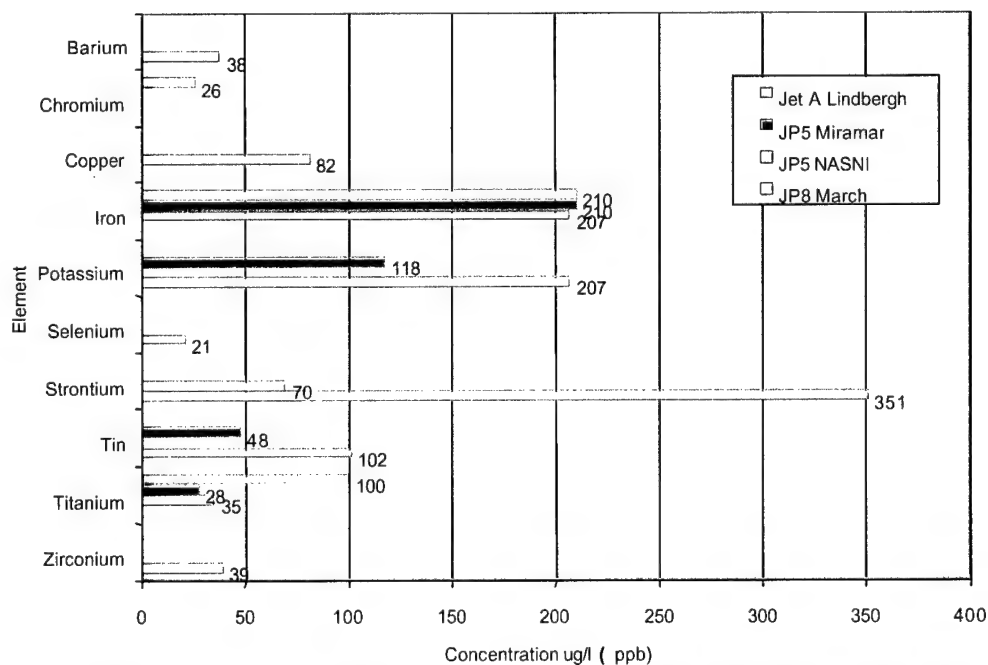


Figure 3. Elements present in concentrations 25 to 400 ppb in jet fuels.

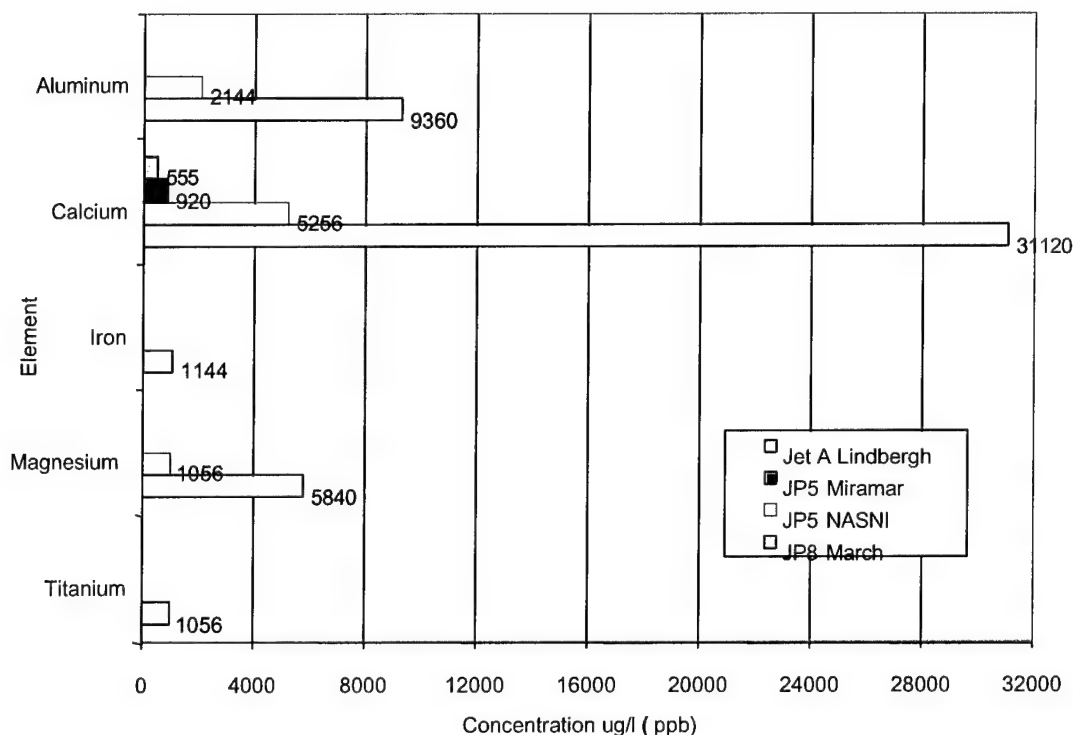


Figure 4. Elements present in concentrations >400 ppb in jet fuels.

The Florida Institute of Technology, Marine and Environmental Chemistry Laboratories⁶ completed a similar, but abbreviated, elemental analysis in 1997 for the Aircraft Environmental Support Office. JP5 and JP8 fuels were analyzed for 13 elements. Table 4 compares results from this study to the 1997 study. Results are reported as “< MDL” in the 1997 study if they were not detected. Results are consistent between the studies.

⁶ “Contaminant Levels in Environmental Samples.” 1997. Technical Report prepared for SSC San Diego by the Florida Institute of Technology, Marine and Environmental Chemistry Laboratories under SSC San Diego Contract Number N66001-96-D-0050: Determination of Contaminant Levels in Environmental Samples.

Table 4. Comparison of jet fuel concentrations with 1997 study.

Element	JP5 in µg/L (ppb)			JP8 in µg/L (ppb)	
	1997 Study	This Study		1997 Study	This Study
		MCAS Miramar	NASNI		
Arsenic	<5	ND	ND	<5	ND
Beryllium	<2	---	---	<2	---
Cadmium	4	ND	ND	8	ND
Chromium	27	9	5	8	18
Copper	18	5	82	6	6
Mercury	<1	ND	ND	<1	ND
Potassium	<100	118	ND	<100	207
Manganese	5	4	10	22	25
Nickel	16	5	6	4	6
Lead	4	2	5	7	10
Selenium	<21	ND	ND	<21	21
Zinc	<50	ND	ND	<50	ND

3.3 POLYCYCLIC AROMATIC HYDROCARBON ANALYSIS

Table 5 compiles the A. D. Little jet fuel PAH analysis results³ and also includes marine diesel and gasoline PAH data from a prior study. The earlier data are compiled from a 1992 SSC San Diego study⁷ of shipboard effluents. Batelle Laboratories performed the analysis. Data from the 1992 report were converted from ng/l to mg/kg using a fuel density of 0.8 kg/l.

Current study results are not blank corrected. Sample results are reported corrected for surrogate recovery. Results found below the minimum reporting limit are qualified as estimated (J). Results found in samples corresponding to a result found in the laboratory procedural blank are qualified with a (B) when the result in the sample is less than five times the result found in the procedural blank. Results found in the blanks were well below the minimum reporting limit. Results not detected are qualified as (ND). Additional qualifiers may be used as defined in the individual data reports or project narrative, and a result may have combinations of these qualifiers (i.e., "JB") Appendix D lists qualifier explanations.

Table 5 PAHs are in order of increasing MW. The higher MW PAHs are generally considered slower to biodegrade and have higher carcinogenic potential. Jet fuel samples had no high MW PAHs present. Gasoline had more mid-range MW (154 to 184) PAHs present than jet fuel, and diesel marine fuel had many more PAHs present and higher concentrations of PAHs.

Benzo[a]pyrene (BAP) is the most studied carcinogenic PAH and is traditionally used as an indicator of overall PAH content. No BAP was detected in the jet fuels.

⁷ B. Chadwick and C. Katz. 1992. "Navy Shipboard Petroleum Hydrocarbon Effluents." Interim report for the Naval Sea Systems Command 5112.

All samples had naphthalene present in the highest concentrations. Naphthalene is the lightest of the PAHs. It biodegrades readily and does not have high carcinogenic potential. Naphthalene concentrations were significantly higher in the Jet A and JP8 fuels than in the JP5 fuels.

Table 5. PAH concentrations in jet fuels.

ID Units		Jet A Lindbergh (mg/kg)	JP5 MCAS Miramar (mg/kg)	JP5 NASNI (mg/kg)	JP8 March AFB (mg/kg)	Gasoline ⁷ (mg/kg)	Marine Diesel ⁷ (mg/kg)
PAH	MW	ppm	ppm	ppm	ppm	ppm	ppm
Napthalene	128	1,900 L	460	540	2,800 L	2,519	1408
C1-Napthalenes		3,900	900	1,100	5,600 L	2,077	5602
C2-Napthalenes		4,900	540	750	3,500	943	13748
C3-Napthalenes		2,700	140	240	380	258	12643
C4-Napthalenes		810	73	92	62	61	8108
Acenaphthylene	152	ND	ND	ND	ND	---	6
Acenaphthene	154	ND	ND	ND	ND	---	---
Biphenyl	154	420	85	110	340	0	---
Fluorene	166	70	8.7	10	5	86	851
C1-Fluorene		56	13	14	2.8J	154	2037
C2-Fluorene		23	17	18	1.6J	135	3585
C3-Fluorene		5.7	9.6	11	ND	58	3175
Anthracene	178	ND	0.47 J	0.57J	ND	8	274
Phenanthrene	178	21	2.6 J	3.8J	0.7J,B	120	2469
C1-Phenanthrenes/ anthracenes		11	4.1J	5.7	0.66J	143	6034
C2-Phenanthrenes/ anthracenes		5	2.7 J	4.6J	ND	76	6126
C3-Phenanthrenes/ anthracenes		1.6J	1.5J	1.5J	ND	19	3045
C4-Phenanthrenes/ anthracenes		ND	ND	ND	ND	---	1056
Dibenzothiophene	184	23	ND	ND	ND	---	1130
C1- Dibenzothiophene		12	0.87J	0.94J	0.46J	---	1779
C2- Dibenzothiophene		4.9	1J	0.9J	ND	---	2881
C3- Dibenzothiophene		2.0 J	ND	ND	ND	0	2122
Fluoranthene	202	ND	0.16 J	0.19 J	ND	16	77
Pyrene		0.24 JB	0.35 JB	0.55 JB	ND	34	172
C1-Fluoranthenes/ pyrenes		ND	ND	ND	ND	32	382
C2-Fluoranthenes/ pyrenes		ND	ND	ND	ND	---	---
C3-Fluoranthenes/ pyrenes		ND	ND	ND	ND	---	---
Benzo[a]anthracene	228	ND	ND	ND	ND	3	5
Chrysene	228	ND	ND	ND	ND	2	15

Table 5. PAH concentrations in jet fuels. (continued)

ID Units		Jet A Lindbergh (mg/kg)	JP5 MCAS Miramar (mg/kg)	JP5 NASNI (mg/kg)	JP8 March AFB (mg/kg)	Gasoline ⁷ (mg/kg)	Marine Diesel ⁷ (mg/kg)
PAH	MW	ppm	ppm	ppm	ppm	ppm	ppm
C1-Chrysene		ND	ND	ND	ND	3	17
C2-Chrysene		ND	ND	ND	ND	---	---
C3-Chrysene		ND	ND	ND	ND	---	---
C4-Chrysene		ND	ND	ND	ND	---	---
Benzo[b]fluor- anthene	252	ND	ND	ND	ND	2	---
Benzo[k]fluor- anthene	252	ND	ND	ND	ND	---	---
Benzo[e]pyrene	252	ND	ND	ND	ND	---	---
Benzo[a]pyrene	252	ND	ND	ND	ND	---	---
Perylene	252	ND	ND	ND	ND	---	---
Indeno[1,2,3,- c,d]pyrene	276	ND	ND	ND	ND	---	---
Dibenzo[a,h]anthra- cene	278	ND	ND	ND	ND	---	---
Benzo[g,h,i]peryl- ene	276	ND	ND	ND	ND	3	---
%d8-Napthalene		110	110	113	115	112	118
%d10-Acenaphthene		103	108	111	111	---	---
%d10- Phenanthrene		106	111	113	112	---	---
%d12- Benzo[a]pyrene		109	108	104	112	---	---

Table 6 compares the results of this study with the JP5 analysis results from the 1992 report.⁷ In the 1992 study, the JP5 was sampled at the San Diego Fleet and Industrial Supply Fuel Farm. Samples were taken in 1990. The right-hand column is the percent change between the 1990 sample and the average of the two recent JP5 samples. Although this is a small data set, PAH values did drop significantly between 1990 and 1999. The phenanthrene measurement was of such low magnitude that it may confirm the presence of the compound, but it is not reliable for quantitative purposes.

Table 6. Comparison of JP5 PAH concentrations with 1992 study.

ID Units	1990 JP5 Study (in mg/kg)	1999 JP5 MCAS Miramar (in mg/kg)	1999 JP5 NASNI (in mg/kg)	1990 versus 1999 % Difference
PAH	ppm	ppm	ppm	ppm
Napthalene	741	460	540	-33%
C1-Napthalenes	1468	900	1100	-32%
C2-Napthalenes	1732	540	750	-63%
C3-Napthalenes	700	140	240	-73%
C4-Napthalenes	173	73	92	-52%
Acenaphthylene	---	ND	ND	---
Acenaphthene	---	ND	ND	---
Biphenyl	---	85	110	---
Fluorene	29	8.7	10	-68
C1-Fluorene	15	13	14	-10%
C2-Fluorene	---	17	18	---
C3-Fluorene	---	9.6	11	---
Anthracene	---	0.47J	0.57J	---
Phenanthrene	1.95	2.6J	3.8J	+64%
C1-Phenanthrens/anthracenes	---	4.1J	5.7	---
C2- Phenanthrens/anthracenes	---	2.7J	4.6J	---
C3- Phenanthrens/anthracenes	---	1.5J	1.5J	---
C4- Phenanthrens/anthracenes	---	ND	ND	---
Dibenzothiophene	---	ND	ND	---
C1- Dibenzothiophene	---	0.87J	0.94J	---
C2- Dibenzothiophene	---	1.0J	0.9J	---
C3- Dibenzothiophene	---	ND	ND	---
Fluoranthene	---	0.16J	0.19J	---
Pyrene	---	0.35J	0.55J	---
C1- Fluoranthenes/pyrenes	---	ND	ND	---
C2- Fluoranthenes/pyrenes	---	ND	ND	---
C3- Fluoranthenes/pyrenes	---	ND	ND	---
Benzo[a]anthracene	---	ND	ND	---
Chrysene	---	ND	ND	---
C1-Chrysene	---	ND	ND	---
C2-Chrysene	---	ND	ND	---
C3-Chrysene	---	ND	ND	---

Table 6. Comparison of JP5 PAH concentrations with 1992 study. (continued)

ID Units	1990 JP5 Study (in mg/kg)	JP5 MCAS Miramar (in mg/kg)	JP5 NASNI (in mg/kg)	1990 versus 1999 % Difference
PAH	ppm	ppm	ppm	ppm
C4-Chrysene	---	ND	ND	---
Benzo[b]fluoranthene	---	ND	ND	---
Benzo[k]fluoranthene	---	ND	ND	---
Benzo[e]pyrene	---	ND	ND	---
Bezno[a]pyrene	---	ND	ND	---
Perylene	---	ND	ND	---
Indeno[1,2,3,-c,d]pyrene	---	ND	ND	---
Dibenzo[a,h]anthracene	---	ND	ND	---
Benzo[g,h,l]perylene	---	ND	ND	---

4. CONCLUSIONS AND REMARKS

In the current study, there were numerous elements and light molecular weight PAHs in the jet fuels. More data sets would help to define a range of typical values and help determine which elements in the fuels are present as delivered from the refinery or introduced as storage and delivery system contaminants. Future analysis efforts should include samples from the refinery.

The average sulfur concentration of 0.02% by weight used in SO₂ emissions calculations for jet engines may need to be revised upwards, per the results of this report.

In the future, the elemental and PAH concentrations in the fuels will be compared to elemental and PAH concentrations in jet engine exhaust particulate matter. Such comparisons may provide insight into how elemental and PAH concentrations in fuel particulates translate to those concentrations in the particulate exhaust after combustion.

5. BIBLIOGRAPHY

Environmental Quality Management, Inc., Roy F. Weston, Inc. 1998. "Aircraft Engine and Auxiliary Power Unit Emissions Testing Report." Draft Scientific and Technical Report prepared under the Air Force Occupational and Environmental Health Assessments Contract F41624-95-D-9019; Volumes 1-4.

U.S. Department of Public Health and Human Services. 1998. "Toxicological Profile for Jet Fuels (JP-5 and JP-8). Report prepared by Research Triangle Institute under Contract 205-93-0606 for The Agency for Toxic Substances and Disease Registry, Atlanta, GA.

U.S. Dept. of Public Health and Human Services. 1998. "Toxicological Profile for Total Petroleum Hydrocarbons." Draft Report prepared by Research Triangle Institute under Contract 205-93-0606 for The Agency for Toxic Substances and Disease Registry, Atlanta, GA.

APPENDIX A
JET FUEL CHEMICAL AND PHYSICAL INFORMATION

3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Information regarding the chemical identities of JP-5 and JP-8 is located in Table 3-1. Information on the composition of jet fuel no. 1 (kerosene) and JP-5 is presented in Table 3-2. Information on the composition of JP-8 is presented in Table 3-3.

Both JP-5 and JP-8 are distillate fuels consisting of distilled process streams refined from crude petroleum. Characteristics of JP-8 fuel (such as density and distillation temperatures) are very similar to those of JP-5 (DOD 1992). There is no standard formula for jet fuels. Their exact composition depends on the crude oil from which they were refined. Variability in fuel composition occurs because of differences in the original crude oil (Custance et al. 1992; IARC 1989) and in the individual additives. As a result of this variability, little information exists on the exact chemical and physical properties of jet fuels (Custance et al. 1992). However, the differences in these fuels are minor. The primary ingredient of both JP-5 and JP-8 is kerosene, and the composition of these fuels is basically the same as kerosene, with the exceptions that they are made under more stringent conditions and contain various additives not found in kerosene (DOD 1992; IARC 1989). The crude oil from which JP-5 and JP-8 are refined is derived from petroleum, tar sands, oil shale, or mixtures thereof (DOD 1992). Typical additives to JP-5 and JP-8 include antioxidants (including phenolic antioxidants), static inhibitors, corrosion inhibitors, fuel system icing inhibitors, lubrication improvers, biocides, and thermal stability improvers (DOD 1992; IARC 1989; Pearson 1988). These additives are used only in specified amounts, as governed by military specifications (DOD 1992; IARC 1989). Straight-run kerosene, the basic component of the kerosene used for jet fuels, consists of hydrocarbons with carbon numbers mostly in the C_9 - C_{14} range. Like all jet fuels, straight-run kerosene consists of a complex mixture of aliphatic and aromatic hydrocarbons (IARC 1989). Aliphatic alkanes (paraffins) and cycloalkanes (naphthenes) are hydrogen saturated, clean burning, and chemically stable and together constitute the major part of kerosene (IARC 1989). Aromatics comprise 10-20% and olefins less than 1% of the jet fuels (IARC 1989). The boiling range of kerosene, JP-5, and JP-8 is well above the boiling point of benzene (a carcinogenic aromatic) and many polycyclic aromatic hydrocarbons (PAHs); consequently, the benzene content of kerosene and these jet fuels is normally below 0.02%, and PAHs are virtually excluded (IARC 1989).

3. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-1. Chemical Identity of JP-5 & JP-8

Characteristic	JP-5	JP-8
Synonym(s)	NATO F-44; AVCAT; MIL-T-5624M; aviation kerosene; kerosene; fuel oil no. 1; jet kerosene; turbo fuel A; straight run kerosene; distillate fuel oils, light ^{a,b,c}	NATO F-34; AVTUR; MIL-T-83133B; aviation kerosene; kerosene; fuel oil no. 1; jet kerosene; turbo fuel A; straight run kerosene; distillate fuel oils, light ^{a,b,c}
Registered trade name(s)	No data	No data
Chemical formula ^d	No data	No data
Chemical structure ^e	No data	No data
Identification numbers:		
CAS registry	8008-20-6 ^f /70892-10-3 ^g	8008-20-6 ^f /70892-10-3 ^g
NIOSH RTECS	QA550000 ^h (kerosene)	QA550000 ^h (kerosene)
EPA hazardous waste	No data	No data
OHM/TADS	7217063 ⁱ (kerosene)	7217063 ⁱ (kerosene)
DOT/UN/NA/IMCO	UN 1223;	UN 1223,
shipping	IMO 3.3 ^b (kerosene)	IMO 3.3 ^b (kerosene)
HSDB	632 ^j	632 ^j (kerosene)
NCI	No data	No data

^aRTECS 1998^bHSDB 1998^cIARC 1989^dArmy 1988^eFuel oils are mixtures of various hydrocarbons designed to meet specifications set forth by the American Society for Testing and Materials (DOD 1992); therefore, chemical structure and chemical formula cannot be determined.^fNTP/NIH 1986^gOHM/TADS 1985

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

3. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-2. Analysis of Fuel Oil No. 1 and JP-5

Hydrocarbon type	Volume %	
	Fuel oil no. 1 ^a	JP-5 ^b
Paraffins (<i>n</i> - and iso-)	52.4	30.6
Monocycloparaffins	21.3	No data
Bicycloparaffins	5.1	No data
Tricycloparaffins	0.8	No data
Total cycloparaffins	27.2	52.8
Total saturated hydrocarbons	79.7	No data
Olefins	No data	0.5
Alkylbenzenes	13.5	No data
Indans/tetralins	3.3	No data
Dinaphthenobenzenes/indenes	0.9	No data
Naphthalenes	2.8	No data
Biphenyls/acenaphthenes	0.4	No data
Fluorenes/acenaphthylenes	No data	No data
Phenanthrenes	No data	No data
Total aromatic hydrocarbons	23.6	15.9

^aDerived from IARC 1989; provided by the American Petroleum Institute^bDerived from sample lot used in NTP/NIH 1986 study

5. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-3. Composition of Surrogate JP-8^a

Hydrocarbon type	Weight %
Isooctane	3.66
Methylcyclohexane	3.51
<i>m</i> -Xylene	3.95
Cyclononane	4.54
Decane	16.08
Butylbenzene	4.72
1,2,4,5-Tetramethylbenzene	4.28
Tetralin	4.14
Dodecane	22.54
1-Methylnaphthalene	3.49
Tetradecane	16.87
Hexadecane	12.22

^aAir Force 1991

2. CHEMICAL AND PHYSICAL INFORMATION

TABLE 3-4. Physical and Chemical Properties of Jet Fuels^a

Characteristic	JP-5	JP-8
Molecular weight ^b	No data	No data
Color	Clear and bright ^c	Clear and bright ^c
Physical state	Liquid ^d	Liquid ^d
Melting point	-56°C ^e	-52°C ^e (sample lot)
Boiling point	170°C ^f 150-290°C ^g	170°C ^f 150-290°C ^g
Density: at 15°C	0.788-0.845 kg/L ⁱ	0.775-0.840 kg/L ⁱ
Odor	Kerosene-like ^h (kerosene)	Kerosene-like ^h (kerosene)
Odor threshold (ppm)	1 ^b , 0.082 ^j (kerosene)	1 ^b , 0.082 ^j (kerosene)
Solubility		
Water at 20°C	~5 mg/L ^d (kerosene)	~5 mg/L ^d (kerosene)
Organic solvent(s)	Miscible with other petroleum solvents ⁱ	Miscible with other petroleum solvents ⁱ
Partition coefficients:		
Log K _{ow}	3.3-7.06 ^e (kerosene)	3.3-7.06 ^e (kerosene)
Log K _{oc}	9.6x10 ³ - 5.5x10 ^{6d} (kerosene)	9.6x10 ³ - 5.5x10 ^{6d} (kerosene)
Vapor pressure at 21°C	2.12-26.4 mmHg ^d (kerosene)	2.12-26.4 mmHg ^d (kerosene)
Henry's law constant		
At 20°C - atm-m ³ /mol	5.9x10 ⁻³ - 7.4 ^d (kerosene)	5.9x10 ⁻³ - 7.4 ^d (kerosene)
Autoignition temperature	229°C ^h (kerosene)	229°C ^h (kerosene)
Flashpoint (minimum)	60°C ^h	38°C ^h
Flammability limits (% volume in air)	0.7%-5% ^h (kerosene)	0.7%-5% ^h (kerosene)
Conversion factors	No data	No data
Explosive limits	0.7%-5% ^h (kerosene)	0.7%-5% ^h (kerosene)

^aValues listed are specifications required or general characteristics of each class of jet fuels.^bFuel oils are mixtures of various hydrocarbons designed to meet specifications set forth by the American Society for Testing and Materials (DOD 1992); therefore, molecular weight cannot be determined.^cDOD 1992^dAir Force 1989b^eAir Force 1989a^fArmy 1988^gTARC 1989^hCoast Guard 1985ⁱOHM/TADS 1985^jHSDB 1998

APPENDIX B

ELEMENTAL ANALYSIS QA/QC DATA²

Element	SRM 1643d This Study (µg/L)	SRM 1643d NIST Certified Mean ± Standard Deviation (µg/L)	SRM Method Detection Limit (µg/L)	Method Spike Recovery (%)	Analytical Spike Recovery (%)	Analytical Precision as RSD of duplicate J2 samples (%)
Ag	1.30	1.270 ±0.057	0.1	104.3	85.1 ± 3.8	N.D.
Al	127	127.6 ±3.5	100	97.9	99.2 ± 0.7	N.D.
As	56.4	56.02 ±0.73	0.2	107.7	137.8 ± 0.6	N.D.
Au	N.D.	-	0.1	100.4	93.7 ± 1.5	N.D.
Ba	507.1	506.5 ±8.9	0.03	103.5	100.0 ± 1.3	15.7
Ca	30.9 mg/L	31.04 ±0.50 mg/L	0.15 mg/L	108.8	106.3 ± 2.9	3.7
Cd	6.50	6.47 ±0.37	0.1	104.5	81.9 ± 1.3	N.D.
Co	24.6	25.00 ±0.59	0.01	102.6	104.7 ± 1.4	N.D.
Cr	18.6	18.53 ±0.20	0.02	102.1	96.9 ± 6.0	6.7
Cu	20.2	20.5 ±3.8	0.02	102.4	107.4 ± 2.9	0.0
Fe	92.2	91.2 ±3.9	0.02	100.0	106.3 ± 2.9	0.3
Ga	N.D.	-	0.5	104.4	105.2 ± 0.9	N.D.
Hg	N.D.	-	0.01	91.5	59.7 ± 4.0	N.D.
K	2.32 mg/L	2.356 ±0.035 mg/L	0.1 mg/L	105.4	104.8 ± 4.3	0.5
Mg	7.81 mg/L	7.989 ±0.035 mg/L	0.1 mg/L	104.7	104.2 ± 3.1	N.D.
Mn	37.1	37.66 ±0.83	0.01	103.1	135.5 ± 2.4	0.0
Mo	112.8	112.9 ±1.7	0.1	103.8	99.7 ± 1.2	N.D.
Ni	56.3	58.1 ±2.7	0.1	104.3	102.7 ± 2.3	0.0
Pb	18.5	18.15 ±0.64	0.05	100.8	99.8 ± 1.0	0.0
Pt	N.D.	-	0.1	-	87.9 ± 3.3	N.D.
Sb	54.5	54.1 ±1.1	0.1	98.9	96.1 ± 0.6	N.D.
Sc	1.1	-	0.5	101.3	113.6 ± 0.4	10.1
Se	11.5	11.43 ±0.17	0.7	100.7	86.0 ± 0.8	N.D.
Sn	3.2	-	0.1	105.7	94.9 ± 2.0	3.6
Sr	292.2	294.8 ±3.4	0.1	102.5	98.5 ± 5.2	7.1
Ti	34.4	-	0.2	99.9	105.8 ± 1.3	2.0
Tl	7.32	7.28 ± 0.25	0.05	101.1	98.7 ± 0.4	N.D.
V	34.3	35.1 ± 1.4	0.1	104.2	106.3 ± 2.1	N.D.
Zn	74	72.48 ± 0.65	20	99.6	96.9 ± 2.9	N.D.
Zr	0.8	-	0.1	102.2	94.0 ± 3.5	4.0

Quality Assurance / Quality Control data for Jet Fuel Analyses: Metal concentrations in SRM 1643d Trace elements in Water certified by the National Institute of Standards and Technology (NIST), SRM Method Detection Limits (MDLs), Method Spike Recoveries, Analytical Spike Recoveries, and Analytical Precision as Percent Relative Standard Deviation (RSD) of duplicate fuel samples.

APPENDIX C
ADL SEMIVOLATILE ORGANICS TARGET, SURROGATE, AND
INTERNAL STANDARD ANALYTE LIST³

Compound	Surrogate Reference	Compound	Surrogate Reference
Napthalene (C0N)	1	Benzo[a]anthracene	3
C1- Napthalene (C1N)	2		
C2- Napthalene (C2N)	2	Chrysene (C0C)	3
C3-Napthalene (C3N)	2	C1-Chrysene (C1C)	3
C4- Napthalene (C4N)	2	C2- Chrysene (C2C)	3
Acenaphthene (ACE)	2	C3- Chrysene (C3C)	4
Acenaphthylene (ACEY)	2	C4- Chrysene (C4C)	4
Biphenyl (BIP)	2	Benzo[b]fluoranthrene	4
Fluorene (C0F)	2	Benzo[k]fluoranthrene	4
C1- Fluorene (C1F)	2	Benzo[a]pyrene	4
C2- Fluorene (C2F)	2	Benzo[e]pyrene	4
C3- Fluorene (C3F)	2	Indeno[1,2,3-c,d]pyrene	4
Dibenzothiophenes (C0D)	3	Dibenzo[a,h]anthracene	4
C1- Dibenzothiophenes	3		
C2- Dibenzothiophenes (C2D)	3		
C3- Dibenzothiophenes (C3D)	3		
Phenanthrene (C0P)	3	Surrogate compounds	
Anthracene (C0A)	3	Napthalene-d8 (D8N)	
C1-	3	Acenaphthene-d10	1,A
C2-	3	Phenanthrene-d10	2,A
C3-	3	Benzo[a]pyrene-d12	3,A
C4-	3		4,B
Fluranthrene (FLANT)	3		
Pyrene (PYR)	3	Recovery Standards	
C1- Fluoranthenes/Pyrenes	3	Fluorene-d10 (D10FL)	
C2- Fluoranthenes/Pyrenes	3	Chrysene-d12 (D12C)	A
C3-Fluoranthenes/Pyrenes	3		B

APPENDIX D

QUALIFIER EXPLANATION³

Qualifier	Explanation
J	Concentrations above zero and below the adjusted minimum reporting limit.
U	Concentration below the adjusted minimum detection limit (MDL).
E	Estimated results exceeds highest level calibration response by greater than 10%.
D	Concentration reported from dilution analysis.
B	Results detected in the associated procedural blank and sample result is less than 5 times the result found in the procedural blank.
I	Estimated result due to interference.
RE	Result reported from a re-analysis for which there is an original result reported.
&	Quality control result exceeds quality control criteria as specified in the laboratory work plan.

Additional qualifiers may be used as defined in the individual data reports or project narrative, and a result may have combinations of these qualifiers, i.e. "JB".

INITIAL DISTRIBUTION

D0012	Patent Counsel	(1)
D0271	Archive/Stock	(6)
D0274	Library	(2)
D027	M. E. Cathcart	(1)
D0271	E. R. Ratliff	(1)
D0271	D. Richter	(1)
D3621	L. A. Shumway	(8)

Defense Technical Information Center
Fort Belvoir, VA 22060-6218 (4)

SSC San Diego Liaison Office
C/O PEO-SCS
Arlington, VA 22202-4804

Center for Naval Analyses
Alexandria, VA 22302-0268

Office of Naval Research
ATTN: NARDIC (Code 362)
Arlington, VA 22217-5660

Government-Industry Data Exchange
Program Operations Center
Corona, CA 91718-8000

Aircraft Environmental Support Office
San Diego, CA 92135-7058 (10)

Air Force Institute for Environment, Safety,
and Occupational Health Risk Analysis
Brooks AFB, TX 78235-5123

U.S. Army Forces Command
Ft. McPherson, GA 30330-6000 (5)

U.S. Environmental Protection Agency
Research Triangle Park, NC 27711 (2)

Florida Institute of Technology
Melbourne, FL 32901-6988

Environmental Quality Management
Cincinnati, OH 45240

Thomas Delmer, Ph.D
La Jolla, CA 92037